

Post-Doctoral Research Fellowships

Applications are open for 1 Post-Doctoral Research Fellowship, within the framework of project “Next-level Artificial Intelligence for heterogeneous catalysis: exploring causal models for the impact of synthesis on catalyst properties”, 2023.12566.PEX, financed by national funds through FCT/MCTES (PIDDAC), under the following conditions:

Scientific Area: Chemistry and Chemical Engineering

Admission Requirements:

- a) *to hold a PhD degree obtained in the 3 years previously to the submission of the fellowship application;*
- b) *to have carried out the research work that led to the PhD degree in a different entity from the host institution of the fellowship;*
- c) *Not to exceed, with this fellowship contract, including the possible renovations, an accumulated period of 3 years in this type of fellowship, continuously or with interruptions;*
- d) *Not to have previously held a post-doctoral fellowship from IST-ID.*

Workplan: The main goal is to develop the first key step of a modelling framework that captures the complexity of a catalytic system, from synthesis to performance, in a single model, suitable for design. This modelling development will rely on existing data for Ni-zeolite catalysts, promising for CO₂ conversion. Therefore, the activities to be carried out are:

- i) Establish a causal diagram (qualitatively describing the effect of synthesis variables on catalyst properties)
- ii) Determine the structural equations (quantifying the effect of synthesis variables on catalyst properties)
- iii) Validate and improve the developed SCM (by comparing with experimental data for Ni-zeolite catalysts)

Profile: Completed PhD degree in Chemical Engineering or equivalent with strong, interdisciplinary background in both experimental catalysis (preferably, on understanding the impact of synthesis on catalyst properties) and machine learning modelling (preferably, causal and/or supervised correlational models).

Legislation and Regulations: Statute of Scientific Research Fellow, approved by Law nr. 40/2004, of August 18, as worded by Decree-Law nr. 123/2019, of August 28; FCT Regulation for Research Studentships and Fellowships, available on <https://www.fct.pt/apoios/bolsas/docs/RegulamentoBolsasFCT2019.pdf> and <https://dre.pt/application/file/a/127230968>.

Working conditions: We offer a multidisciplinary working environment with excellent potential for scientific and personal development integrated in the [Digital Catalysis group](#). At DigiCat, we strive for wellbeing and work-life balance as key feature of an integral scientific venture. The student will be provided with high-performance laptop and all necessary office supplies. Training and conference expenses will be entirely covered by the project. Stays abroad are possible, but not mandatory. Hybrid working mode is possible, but not mandatory.

Workplace: The work will be developed at the [Digital Catalysis group](#) of [Centro de Química Estrutural](#) of Instituto Superior Técnico, under the scientific supervision of Prof. Pedro Mendes.



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Duration: The research fellowship will have the duration of 10 months. It's expected to begin in September 2025, and may be eventually renewed up to the maximum of 6 months.

Monthly maintenance allowance: According to the values for Research Fellowships awarded by FCT in Portugal (<https://www.fct.pt/fct-atualizou-o-valor-das-bolsas-para-2025/>), the amount of the monthly maintenance allowance is € 1851, being the payment method of the Fellow by wire transfer.

Selection methods: The selection criteria will be the following:

- 40 % *Overall quality and diversity of experiences in the academic and career path*
- 30 % *Specific skills on catalyst synthesis and characterization, and machine learning*
- 30 % *Soft skills on teamwork, proactiveness, and inclusivity.*

The jury might select upon three candidates for a brief discussion. This will uniquely aim at clarify particular aspects related to the selection criteria above, not being a criterion on its own.

Composition of the selection Jury: Prof. Pedro Mendes, Prof. Catarina Barata, Dr. Carmen Bacariza.

Announcement/ notification of the results: The final evaluation results will be communicated to all applicants by email.

Deadlines and procedures of complaint and appeal. A complaint may be lodged from the final decision within 15 working days, or an appeal to the Executive Board of IST-ID within 30 working days, both counted from the respective notification.

Application deadline and formalization: The call is open from June 16 until June 30, 2025.

It is mandatory to formalize applications with the submission of the following documents: i) B1 Form – Fellowship application (<https://ist-id.pt/concursos/bolsas/>); ii) *Curriculum Vitae*; iii) academic degree certificate; iv) motivation letter; v) declaration on honour that the applicant does not exceed with this contract an accumulated period of three years in this type of fellowship, continuously or with interruptions, within the technological and scientific system, and that the research work that led to the PhD degree was carried out in a different entity from the host institution of the fellowship.

Applications must be submitted to the email: digicat@tecnico.ulisboa.pt



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